Distance bounds on quantum dynamics

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We derive rigorous upper bounds on the distance between quantum states in an open-system setting in terms of the operator norm between Hamiltonians describing their evolution. We illustrate our results with an example taken from protection against decoherence using dynamical decoupling.

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I. INTRODUCTION

When an open quantum system undergoes a dynamical evolution generated by a Hamiltonian, how far does its state evolve from itself compared to the magnitude of the Hamiltonian? This is a fundamental question that is central to quantum-information science [1] and quantum control [2,3]. In order to make it more precise, suppose that the unitary propagator of the evolution, $U(t)$, which is related to the Hamiltonian $H(t)$ via the Schrödinger equation $\dot{U}=-\frac{i}{\hbar}HU$, is written in terms of an effective Hamiltonian $\Omega(t)$ as $U(t)=\exp[-it\Omega(t)/\hbar]$. The effective Hamiltonian can in turn by calculated from the Hamiltonian $H(t)$ using a Dyson or Magnus expansion. If the system S is "open," it is coupled to a bath B and its time-evolved state is given via the partial trace operation by $\rho_S(t)=\mathrm{Tr}_B\, U(t)\rho(0)U(t)^\dagger$ [4,5]. In the context of quantum information, the question we have stated pertains to the problem of "quantum memory": i.e., what is $\|\rho_S(t)-\rho_S(0)\|$ compared to $\|\Omega(t)\|$ or $\|H(t)\|$? When the issue is quantum computation or general quantum control, one is interested in comparing two time-evolved states: the "ideal" state $\rho_S^0(t)$, which is error free and is described by an "ideal" effective Hamiltonian $\Omega^0(t)$ (e.g., for a quantum algorithm), and the "actual" state $\rho_S(t)$, which undergoes the full noisy dynamics described by the total effective Hamiltonian $\Omega(t)$. Then the question becomes the following: what is $\|\rho_S(t)-\rho_S^0(t)\|$ compared to $\|\Omega(t)-\Omega^0(t)\|$ or $\|H(t)-H^0(t)\|$? The memory question can, of course, be seen as a special case of the computation question.

Here we prove bounds that answer these fundamental questions. Our bounds have immediate applications to problems in decoherence control [6] and fault-tolerant quantum computation [7], as they quantify the sense in which a distance between (effective) Hamiltonians describing the evolution should be made small, in order to guarantee a small distance between a desired and actual state.

To begin, we first recall the definition and key properties of so-called unitarily invariant norms, as we use such norms extensively (Sec. II). We mention the trace norm and operator norm, and a norm that mixes them via a duality between the Schrödinger and Heisenberg pictures. We then briefly review the accepted distance measures between states so as to quantify the meaning of an expression such as $\|\rho_S(t)-\rho_S^0\|(t)$ (Sec. III). Next, we discuss how to compute the effective Hamiltonian $\Omega(t)$ using the Magnus expansion or Thompson's theorem, and introduce a generalized effective superoperator generator (Sec. IV). Since in many applications one is interested not in the distance between states generated by unitary, closed-system evolution, but instead in the distance between states of systems undergoing nonunitary, open-system dynamics, we prove an upper bound on the distance between such system-only states in terms of the distance between the full "system+bath" states (Sec. V). We then come to our main result: an upper bound on the distance between system states in terms of the distance between (effective) Hamiltonians describing the system+bath dynamics (Sec. VI). We find the intuitive result that the distance is upper bounded by a function depending on the spectral diameter of the difference between the effective Hamiltonians. We present a discussion of our result in terms of an example borrowed from decoherence control using dynamical decoupling (Sec. VII). We conclude in Sec. VIII with some open questions.

II. UNITARILY INVARIANT NORMS

Unitarily invariant norms are norms satisfying, for all unitary U,V [8],

$$\|UAV\|_{\mathrm{ui}}=\|A\|_{\mathrm{ui}}. \tag{1}$$

We list some important examples.

(i) The trace norm:

$$\|A\|_1 \equiv \mathrm{Tr}|A| = \sum_i s_i(A), \tag{2}$$

where $|A| \equiv \sqrt{A^\dagger A}$ and $s_i(A)$ are the singular values (eigenvalues of $|A|$).

(ii) The operator norm: Let $\mathcal{V}$ be an inner product space equipped with the Euclidean norm $\|x\| \equiv \sqrt{\sum_i |x_i|^2 \langle e_i, e_i \rangle}$, where $x = \sum_i x_i e_i \in \mathcal{V}$ and $\mathcal{V} = \mathrm{Sp}\{e_i\}$. Let $\Lambda : \mathcal{V} \mapsto \mathcal{V}$. The operator norm is

$$\|\Lambda\|_\infty \equiv \sup_{x \in V} \frac{\|\Lambda x\|}{\|x\|} = \max_i s_i(\Lambda). \tag{3}$$

Therefore $\|\Lambda x\| \le \|\Lambda\|_\infty \|x\|$. In our applications $\mathcal{V} = \mathcal{L}(\mathcal{H})$ is the space of all linear operators on the Hilbert space $\mathcal{H}$, Λ is a superoperator, and $x = \rho$ is a normalized quantum state: $\|\rho\|_1 = \mathrm{Tr}\,\rho = 1$.

(iii) The Frobenius, or Hilbert-Schmidt, norm:

$$\|A\|_2 \equiv \sqrt{\mathrm{Tr}\, A^\dagger A} = \sqrt{\sum_i s_i(A)^2}. \tag{4}$$

All unitarily invariant norms satisfy the important property of submultiplicativity [9]:

$$\|AB\|_{\mathrm{ui}} \le \|A\|_{\mathrm{ui}} \|B\|_{\mathrm{ui}}. \tag{5}$$

The norms of interest to us are also multiplicative over tensor products and obey an ordering [9]

$$\|A \otimes B\|_i = \|A\|_i \|B\|_i, \quad i = 1, 2, \infty,$$

$$\|A\|_\infty \le \|A\|_2 \le \|A\|_1,$$

$$\|AB\|_{\mathrm{ui}} \le \|A\|_\infty \|B\|_{\mathrm{ui}}, \|B\|_\infty \|A\|_{\mathrm{ui}}. \tag{6}$$

There is an interesting duality between the trace and operator norm [9]:

$$\|A\|_1 = \max\{|\mathrm{Tr}(B^\dagger A)| : \|B\|_\infty \le 1\}, \tag{7}$$

$$\|A\|_\infty = \max\{|\mathrm{Tr}(B^\dagger A)| : \|B\|_1 \le 1\}, \tag{8}$$

$$|\mathrm{Tr}(BA)| \le \|A\|_\infty \|B^\dagger\|_1, \|B^\dagger\|_\infty \|A\|_1. \tag{9}$$

In the last three inequalities A and B can map between spaces of different dimensions. If they map between spaces of the same dimension, then

$$\|A\|_1 = \max_{B^\dagger B = I} |\mathrm{Tr}(B^\dagger A)|. \tag{10}$$

We now define another norm, which we call the "operator-trace" norm (O-T norm):

$$\|\Lambda\|_{\infty,1} \equiv \sup_{\rho \in \mathcal{L}(\mathcal{H})} \frac{\|\Lambda\rho\|_1}{\|\rho\|_1} = \sup_{\|\rho\|_1 = 1} \|\Lambda\rho\|_1, \tag{11}$$

where $\Lambda : \mathcal{V} \mapsto \mathcal{V}$ and $\mathcal{V}$ is a normed space equipped with the trace norm. Note that if $\Lambda\rho$ is another normalized quantum state, then $\|\Lambda\|_{\infty,1} = 1$. Also, by definition, $\|\Lambda\rho\|_1 \le \|\Lambda\|_{\infty,1}$. Moreover, it follows immediately from the unitary invariance of the trace norm that the OT norm is unitarily invariant. Indeed, let $\Gamma \cdot = V \cdot V^\dagger$ be a unitary superoperator (i.e., V is unitary); then, $\|\Gamma_1 \Lambda \Gamma_2^\dagger\|_{\infty,1} = \sup_\rho \|V_2 V_1 (\Lambda\rho) V_1^\dagger V_2^\dagger\|_1 = \sup_\rho \|\Lambda\rho\|_1 = \|\Lambda\|_{\infty,1}$. Therefore the OT norm is also submultiplicative. However, note that unlike the case of the standard operator norm, there is no simple expression for $\|\Lambda\|_{\infty,1}$ in terms of the singular values of Λ.

On the other hand, if Λ_* denotes the Hilbert-Schmidt dual of Λ, i.e.,

$$\mathrm{Tr}[\Lambda(\rho)X] = \mathrm{Tr}[\rho\Lambda_*(X)] \quad \forall\, \rho, X, \tag{12}$$

then one can prove the following identity [see, e.g., Sec. 2.4 of Ref. [10] or Eq. (9) of Ref. [11]]:

$$\|\Lambda\|_{\infty,1} = \|\Lambda\|_{*\infty} := \sup_{\|X\|_\infty = 1} \|\Lambda_*(X)\|_\infty = \max_i s_i(\Lambda_*). \tag{13}$$

For example, for completely positive maps [1,4,5] $\Lambda\rho = \sum_i A_i \rho A_i^\dagger$ (where $\{A_i\}$ are the Kraus operators), it is easily verified that $\Lambda_*\rho = \sum_i A_i^\dagger \rho A_i$. The duality (12) between Λ and Λ_* is the duality between the Heisenberg and Schrödinger pictures.

III. DISTANCE AND FIDELITY MEASURES

Various measures are known that quantify the notion of distance and fidelity between states. For example, the distance measure between quantum states ρ_1 and ρ_2 is the trace distance

$$D(\rho_1, \rho_2) \equiv \frac{1}{2}\|\rho_1 - \rho_2\|_1. \tag{14}$$

The trace distance is the maximum probability of distinguishing ρ_1 from ρ_2: namely, $D(\rho_1, \rho_2) = \max_{0<P<I}(\langle P\rangle_1 - \langle P\rangle_2)$, where $\langle P\rangle_i = \mathrm{Tr}\,\rho_i P$ and P is a projector, or more generally an element of a positive operator-valued measure (POVM) [1]. The fidelity between quantum states ρ_1 and ρ_2 is

$$F(\rho_1, \rho_2) \equiv \|\sqrt{\rho_1}\sqrt{\rho_2}\|_1 = \sqrt{\sqrt{\rho_1}\rho_2\sqrt{\rho_1}}, \tag{15}$$

which reduces for pure states $\rho_1 = |\psi\rangle\langle\psi|$ and $\rho_2 = |\phi\rangle\langle\phi|$ to $F(|\psi\rangle, |\phi\rangle) = |\langle\psi|\phi\rangle|$. The fidelity and distance bound each other from above and below [12]:

$$1 - D(\rho_1, \rho_2) \le F(\rho_1, \rho_2) \le \sqrt{1 - D(\rho_1, \rho_2)^2}, \tag{16}$$

so that knowing one bounds the other. Many other measures exist and are useful in a variety of circumstances [1].

IV. GENERATORS OF THE DYNAMICS

A. Effective superoperator generators

We shall describe the evolution in terms of an effective superoperator generator $L(t)$, such that

$$\rho(0) \mapsto \rho(t) \equiv e^{tL(t)}\rho(0). \tag{17}$$

The advantage of this general formulation is that it incorporates nonunitary evolution as well. Nevertheless, here we focus primarily on the case of unitary evolution $\rho(t) = U(t)\rho(0)U(t)^\dagger$, with $\dot{U} = -\frac{i}{\hbar}HU$, for which we have

$$L(t) = -\frac{i}{\hbar}[\Omega(t),\cdot]. \tag{18}$$

This follows immediately from the identity $e^{-iA}\rho e^{iA} = e^{-i[A,\cdot]}\rho \equiv \sum_{n=0}^{\infty}\frac{(-i)^n}{n!}[_nA,\rho]$, satisfied for any Hermitian operator A, where $[_nA,\rho]$ denotes a nested commutator—i.e., $[_nA,\rho]=[A,[_{n-1}A,\rho]]$—with $[_0A,\rho]\equiv\rho$.

B. Magnus expansion

In perturbation theory the effective Hamiltonian can be evaluated most conveniently by using the Magnus expansion, which provides a unitary perturbation theory, in contrast to the Dyson series [13]. The Magnus expansion expresses $\Omega(t)$ as an infinite series: $\Omega(t)=\sum_{n=1}^{\infty}\Omega_n(t)$, where $\Omega_1(t)=\frac{1}{t}\int_0^t H(t_1)dt_1$ and the nth-order term involves an integral over an nth-level nested commutator of $H(t)$ with itself at different times. A sufficient (but not necessary) condition for absolute convergence of the Magnus series for $\Omega(t)$ in the interval $[0,t)$ is [14]

$$\int_0^t H(s)_\infty ds < \pi. \tag{19}$$

C. Relating the effective Hamiltonian to the "real" Hamiltonian

There is also a way to relate the effective Hamiltonian to the real Hamiltonian in a nonperturbative manner. To this end we make use of a recently proven theorem due to Thompson [15,16].

Let us consider a general quantum evolution generated by a time-dependent Hamiltonian H, where V is considered a perturbation to H_0 (in spite of this we will not treat V perturbatively):

$$H(t) = H_0(t) + V(t). \tag{20}$$

The propagators satisfy

$$\frac{dU(t,0)}{dt} = -iH(t)U(t,0), \tag{21}$$

$$\frac{dU_0(t,0)}{dt} = -iH_0(t)U_0(t,0). \tag{22}$$

We define the interaction picture propagator with respect to H_0, as usual, via

$$\tilde{U}(t,0) = U_0(t,0)^\dagger U(t,0). \tag{23}$$

It satisfies the Schrödinger equation

$$\frac{d\tilde{U}(t,0)}{dt} = -i\tilde{H}(t)\tilde{U}(t,0), \tag{24}$$

with the interaction picture Hamiltonian

$$\tilde{H}(s) = U_0(t,0)^\dagger V(t)U_0(t,0). \tag{25}$$

See Appendix A for a proof.

The interaction picture propagator $\tilde{U}(t,0)$ can be formally expressed as

$$\tilde{U}(t,0) = \mathcal{T}[\exp(-i\int_0^t \tilde{H}(s)ds)] \tag{26}$$

$$\equiv \exp[-it\tilde{\Omega}(t)], \tag{27}$$

where the second equality serves to define the effective interaction picture Hamiltonian $\tilde{\Omega}(t)$.

Lemma 1. There exist unitary operators $\{W(s)\}$ such that

$$\tilde{\Omega}(t) \equiv \frac{1}{t}\int_0^t W(s)\tilde{H}(s)W(s)^\dagger ds. \tag{28}$$

This is remarkable since it shows that the time-ordering problem can be converted into the problem of finding the (continuously parametrized) set of unitaries $\{W(s)\}$.

Proof. The formal solution (26) can be written as an infinite, ordered product

$$\tilde{U}(t,0) = \lim_{N\to\infty}\prod_{j=0}^{N}\exp\left[-i\frac{t}{N}\tilde{H}\left(\frac{jt}{N}\right)\right]. \tag{29}$$

Thompson's theorem [15,16] states that for any pair of operators A and B, there exist unitary operators V and W, such that $e^Ae^B=e^{VAV^\dagger+WBW^\dagger}$. It follows immediately that if $\{A_j\}_{j=0}^N$ are Hermitian operators, then it is always possible to find unitary operators $\{W_j\}_{j=1}^N$ such that

$$\prod_{j=0}^{N}\exp[-iA_j] = \exp[-i\sum_{j=0}^{N}W_jA_jW_j^\dagger]. \tag{30}$$

The proof is nonconstructive, i.e., the unitary operators $\{W_j\}_{j=1}^N$ are not known. Applying this to Eq. (29) yields

$$\tilde{U}(t,0) = \lim_{N\to\infty}\exp\left[-i\frac{t}{N}\sum_{j=0}^{N}W_j\tilde{H}\left(\frac{jt}{N}\right)W_j^\dagger\right]$$
$$= \exp[-i\int_0^t W(s)\tilde{H}(s)W(s)^\dagger ds], \tag{31}$$

which is the claimed result with the effective Hamiltonian $\tilde{\Omega}(t)$ defined as in Eq. (28). ■

An immediate corollary of Lemma 1 is the following:

Corollary 1. The effective Hamiltonian $\tilde{\Omega}(t)$ defined in Eq. (28) satisfies, for any unitarily invariant norm,

$$\|\tilde{\Omega}(t)\|_{\text{ui}} \le \frac{1}{t}\int_0^t ds\|V(s)\|_{\text{ui}} \equiv \langle\|V\|_{\text{ui}}\rangle \tag{32}$$

$$\le \sup_{0<s<t}\|V(s)\|_{\text{ui}}. \tag{33}$$

Proof. We have [Eq. (25)] $\tilde{H}(s)=U_0(t,0)^\dagger V(t)U_0(t,0)$ and [Eq. (28)] $\|\tilde{\Omega}(t)\|_{\text{ui}}=\|\frac{1}{t}\int_0^t W(s)\tilde{H}(s)W(s)^\dagger ds\|_{\text{ui}}$. The result follows from the triangle inequality. ■

We have presented the bound in the interaction picture. Clearly, the same argument applies to the Schrödinger picture, where instead one obtains

$$\|\Omega(t)\|_{\mathrm{ui}} \le \frac{1}{t}\int_0^t ds\|H_0(s)+V(s)\|_{\mathrm{ui}}. \tag{34}$$

V. DISTANCE BEFORE AND AFTER PARTIAL TRACE

Since we are interested in the distances between states undergoing open system dynamics, we now prove the following.

Lemma 2. Let $\mathcal{H}_S$ and $\mathcal{H}_B$ be finite-dimensional Hilbert spaces of dimensions d_S and d_B, and let $A \in \mathcal{H}_S \otimes \mathcal{H}_B$. Then for any unitarily invariant norm that is multiplicative over tensor products the partial trace satisfies the norm inequality

$$\|\mathrm{tr}_B\, A\| \le \frac{d_B}{\|I_B\|}\|A\|, \tag{35}$$

where I is the identity operator.

This result was already known for the trace norm as a special case of the contractivity of trace-preserving quantum operations [1].

Proof. Consider a unitary irreducible representation $\{U_B(g), g \in G\}$ of a compact group G on $\mathcal{H}_B$. Then it follows from Schur's lemma that the partial trace has the following representation [17]:

$$\frac{1}{d_B}\mathrm{tr}_B(X)\otimes I_B = \int_G [I_A \otimes U_B(g)]X[I_A \otimes U_B(g)^\dagger]d\mu(g), \tag{36}$$

where $d\mu(g)$ denotes the left-invariant Haar measure normalized as $\int_G d\mu(g)=1$ and $d_B \equiv \dim(\mathcal{H}_B)$. Then

$$\begin{aligned}\|\mathrm{tr}_B\, X\| &= \frac{1}{\|I_B\|}\|\mathrm{tr}_B(X)\otimes I_B\| \\ &\le \frac{d_B}{\|I_B\|}\int_G \|[I_A\otimes U_B(g)]X[I_A\otimes U_B(g)^\dagger]\|d\mu(g) \\ &= \frac{d_B}{\|I_B\|}\int_G \|X\|d\mu(g) = \frac{d_B}{\|I_B\|}\|X\|. \end{aligned}\tag{37}$$

■

In particular, $\|I_B\|_1=d_B$, $\|I_B\|_2=\sqrt{d_B}$, and $\|I_B\|_\infty=1$, and since the trace, Frobenius, and operator norms are all multiplicative over tensor products, we have, specifically,

$$\|\mathrm{tr}_B\, X\|_1 \le \|X\|_1, \tag{38}$$

$$\|\mathrm{tr}_B\, X\|_2 \le \sqrt{d_B}\|X\|_2, \tag{39}$$

$$\|\mathrm{tr}_B\, X\|_\infty \le d_B\|X\|_\infty. \tag{40}$$

Note that not all unitarily invariant norms are multiplicative over tensor products. For instance, the Ky-Fan k norm $\|\cdot\|_{(k)}$ is the sum of the k largest singular values and is unitarily invariant [8], but it is not multiplicative in this way. For example, when $d_A=d_B=d\ge k\ge 2$ we have $\|I_A\|_{(k)}=\|I_B\|_{(k)}=\|I_A\otimes I_B\|_{(k)}=k$. So for $X=I_A\otimes I_B$ we have $\|\mathrm{tr}_B X\|_{(k)}=d\|I_A\|_{(k)}=dk$, but $(d_B/\|I_B\|_{(k)})\|X\|_{(k)}=(d/k)k=d$, which gives an inequality in the wrong direction.

VI. DISTANCE BOUND

We are now ready to prove our main theorem, which provides a bound on the distance between states in terms of the distance between effective superoperator generators. As an immediate corollary, we obtain the bound in terms of the effective Hamiltonians.

How much does the deviation between $L(t)$ and $L^0(t)$ impact the deviation between $\rho(t)$ and $\rho^0(t)$? We shall assume that the desired evolution is unitary—i.e., $e^{tL^0(t)}=U^0(t)\cdot U^0(t)^\dagger$, where $U^0(t)=e^{-\frac{i}{\hbar}t\Omega^0(t)}$.

Theorem 1. Consider two evolutions: the "desired" unitary evolution $\rho(0)\mapsto\rho^0(t)\equiv e^{tL^0(t)}\rho(0)=e^{-(i/\hbar)t[\Omega^0(t),\cdot]}\rho(0)$ and the "actual" evolution $\rho(0)\mapsto\rho(t)\equiv e^{tL(t)}\rho(0)$. Let $\Delta L(t)\equiv L(t)-L^0(t)$. Then

$$D[\rho(t),\rho^0(t)] \le \min\left[1,\frac{1}{2}(e^{t\|\Delta L(t)\|_{\infty,1}}-1)\right].$$

If in addition $t\|\Delta L(t)\|_{\infty,1}\le 1$, then

$$D[\rho(t),\rho^0(t)] \le t\|\Delta L(t)\|_{\infty,1}.$$

Note that, using the Heisenberg-Schrödinger duality (13), we can replace $\|\Delta L(t)\|_{\infty,1}$ by $\|\Delta L_*(t)\|_\infty$, where ΔL_* is the dual generator to ΔL. In the case of Hamiltonian evolution we can make this explicit as follows.

Corollary 2. For Hamiltonian evolution, where $L(t)=-\frac{i}{\hbar}[\Omega(t),\cdot]$ and $L^0(t)=-\frac{i}{\hbar}[\Omega^0(t),\cdot]$, and defining the spectral diameter $\Delta\lambda(t)\equiv\max_{i,j}|\lambda_i(t)-\lambda_j(t)|=\max_i\lambda_i(t)-\max_i\lambda_i(t)$, where $\{\lambda_i(t)\}$ are the eigenvalues of $\Delta\Omega(t)\equiv\Omega(t)-\Omega^0(t)$,

$$D[\rho(t),\rho^0(t)] \le \min\left[1,\frac{1}{2}(e^{t\,\Delta\lambda(t)/\hbar}-1)\right] \tag{41}$$

$$\le t\,\Delta\lambda(t)/\hbar \quad \text{if } t\,\Delta\lambda(t)/\hbar \le 1. \tag{42}$$

Corollary 2 means that the "spectral action" $t\,\Delta\lambda(t)/\hbar$ plays a key role in bounding the distance between states, a pleasingly intuitive result.

Proof of Theorem 1. Let us define Hermitian operators

$$\mathcal{H}^0 \equiv itL^0(t), \quad \mathcal{H}\equiv itL(t), \tag{43}$$

and consider (superoperator) unitaries generated by these operators as a function of a new time parameter s (we shall hold t constant):

$$d\mathcal{U}_0/ds = -i\mathcal{H}^0\mathcal{U}_0, \quad d\mathcal{U}/ds=-i\mathcal{H}\mathcal{U}. \tag{44}$$

Then

$$\mathcal{U}_0(s)=e^{-is\mathcal{H}^0}, \quad \mathcal{U}(s)=e^{-is\mathcal{H}}, \tag{45}$$

and we can define an interaction picture via

$$\mathcal{U}(s)=\mathcal{U}_0(s)\mathcal{S}(s), \tag{46}$$

where the interaction picture "perturbation" is

$$\tilde{V}(s) \equiv \mathcal{U}_0^\dagger(s)(\mathcal{H}-\mathcal{H}^0)\mathcal{U}_0(s) = it\mathcal{U}_0^\dagger(s)\Delta L(t)\mathcal{U}_0(s). \quad (47)$$

Then, using (1) unitary invariance and (2) the definition of the $\| \|_{\infty,1}$ norm [Eq. (11)],

$$D[\rho(t),\rho^0(t)] = \frac{1}{2}\|e^{tL^0(t)}(e^{-tL^0(t)}e^{tL(t)}-\mathcal{I})\rho(0)\|_1 \overset{(1)}{=} \frac{1}{2}\|(\mathcal{S}(1)-\mathcal{I})\rho(0)\|_1 \overset{(2)}{\leq} \frac{1}{2}\|\mathcal{S}(1)-\mathcal{I}\|_{\infty,1}, \quad (48)$$

which explains why we introduced $\mathcal{S}$. We can compute $\mathcal{S}$ using the Dyson series of time-dependent perturbation theory:

$$d\mathcal{S}/ds = -i\tilde{V}\mathcal{S},$$

$$\mathcal{S}(s) = \mathcal{I} + \sum_{m=1}^{\infty}\mathcal{S}_m(s),$$

$$\mathcal{S}_m(s) = \int_0^s ds_1 \int_0^{s_1} ds_2 \int_0^{m-1} ds_m \tilde{V}(s_1)\tilde{V}(s_2)\cdots\tilde{V}(s_m). \quad (49)$$

Using submultiplicativity and the triangle inequality, we can then show that (see Appendix B for the details)

$$\|\mathcal{S}(s)-\mathcal{I}\|_{\infty,1} \leq e^{\|t\,\Delta L(t)s\|_{\infty,1}} - 1. \quad (50)$$

Thus, finally, we have from Eq. (48)

$$D[\rho(t),\rho^0(t)] \leq \frac{1}{2}(e^{\|t\,\Delta L(t)\|_{\infty,1}} - 1). \quad (51)$$

If additionally $t\|\Delta L\|_{\infty,1} \leq 1$, then the inequality $e^x - 1 \leq (e-1)x$ yields $D[\rho(t),\rho^0(t)] \leq t\|\Delta L(t)\|_{\infty,1}$. On the other hand, note that $D[\rho(t),\rho^0(t)] = \frac{1}{2}\|[\mathcal{S}(1)-\mathcal{I}]\rho(0)\|_1 \leq \frac{1}{2}[\|\mathcal{S}(1)\rho(0)\|_1 + \|\rho(0)\|_1] = 1$. ■

Proof of Corollary 2. For Hamiltonian evolution we have

$$\hbar\|\Delta L(t)\|_{\infty,1} = \|[\Delta\Omega(t),\cdot]\|_{\infty,1} \overset{(1)}{=} \|[\Delta\Omega(t),\cdot]_*\|_\infty \overset{(2)}{=} \|[\Delta\Omega(t),\cdot]\|_\infty = \max_{i,j}|\lambda_i(t)-\lambda_j(t)| \equiv \Delta\lambda(t), \quad (52)$$

where $\{\lambda_i\}$ are the eigenvalues of $\Delta\Omega$. To obtain this result we used (a) Eq. (13) and (b) the duality relation (12), which yields $\mathrm{Tr}([\Delta\Omega,\rho]_* X) = \mathrm{Tr}(\rho[\Delta\Omega,X]) = \mathrm{Tr}([-\Delta\Omega,\rho]X)\ \forall \rho, X$, and hence $[\Delta\Omega,\cdot]_* = [-\Delta\Omega,\cdot]$. ■

VII. DISCUSSION

A. General bound

By putting together Eq. (35) and Corollary 2, we can answer the question we posed in the Introduction.

Theorem 2. Consider a quantum system S coupled to a bath B, undergoing evolution under either the "actual" joint unitary propagator $U(t) = e^{-i/\hbar t\Omega(t)}$ or the "desired" joint unitary propagator $U^0(t) = e^{-i/\hbar t\Omega^0(t)}$, generated, respectively, by $H(t)$ and $H^0(t)$. Let $\Delta\lambda(t)$ denote the spectral diameter of $\Omega(t)-\Omega^0(t)$. Then the trace distance between the actual time-evolved system state $\rho_S(t) = \mathrm{tr}_B U(t)\rho(0)U(t)^\dagger$ and the desired one $\rho_S^0(t) = \mathrm{tr}_B U^0(t)\rho(0)U^0(t)^\dagger$ satisfies the bound

$$D[\rho_S(t),\rho_S^0(t)] \leq \min\left[1, \frac{1}{2}(e^{t\,\Delta\lambda(t)/\hbar} - 1)\right] \quad (53)$$

$$\leq \min\left[1, \frac{1}{2}(e^{(2/\hbar)[\langle\|\Delta H(t)\|_\infty\rangle]} - 1)\right], \quad (54)$$

where $\langle\|X\|_\infty\rangle \equiv \frac{1}{t}\int_0^t ds\|X(s)\|_\infty$ and $\Delta H(t)$ is the Hamiltonian generating $U_\Delta(t) \equiv e^{-(i/\hbar)t\,\Delta\Omega(t)}$.

To obtain the second inequality we used $\Delta\lambda(t) = \|[\Delta\Omega(t),\cdot]\|_\infty \leq 2\|\Delta\Omega(t)\|_\infty$ and Corollary 1.

Theorem 2 shows that to minimize the distance between the actual and desired evolution it is sufficient to minimize the spectral diameter of the actual and desired effective Hamiltonians, or the time average of the operator norm of the difference Hamiltonian ΔH. Techniques for doing so which explicitly use the Magnus expansion or operator norms include dynamical decoupling [18,19] and quantum error correction for non-Markovian noise [20–24].

B. Illustration using concatenated dynamical decoupling

As an illustration, consider the scenario of a single qubit coupled to a bath via a general system-bath Hamiltonian $H_{SB} = H_S \otimes I_B + \Sigma_{\alpha=x,y,z}\sigma_\alpha \otimes B_\alpha$ (H_S is the system-only Hamiltonian, σ_α are the Pauli matrices, and $B_\alpha \neq I_B$ are bath operators), with a bath Hamiltonian H_B and controlled via a system Hamiltonian $H_C(t)$, so that the total Hamiltonian is $H(t) = H_C(t)\otimes I_B + H_{SB} + I_S \otimes H_B$. Suppose that one wishes to preserve the state of the qubit—i.e., we are interested in "quantum memory"—so that $\Omega^0(t) = H_C(t)\otimes I_B + I_S \otimes H_B$. It was shown in Ref. [19], Eq. (51), that by using concatenated dynamical decoupling (a recursively defined pulse sequence [25]) and assuming zero-width pulses, the Magnus expansion yields the following upper bound:

$$T\|\Omega(T)-\Omega^0(T)\|_{\mathrm{ui}}/\hbar \leq JT(\beta T/N^{1/2})^{\log_4 N}. \quad (55)$$

Here $\Omega(t)$ is the effective Hamiltonian corresponding to the evolution generated by $H(t)$, $T = N\tau$ (the duration of a concatenated pulse sequence with pulse interval τ), and

$$\beta \equiv \|H_B\|_{\mathrm{ui}}, \quad J \equiv \max_\alpha \|B_\alpha\|_{\mathrm{ui}} \quad (56)$$

are measures of the bath and system-bath coupling strength, respectively. Here we shall take the norm in these last two definitions as the operator norm. The bound (55) is valid as long as $\beta T \ll 1$ [19]. When this is the case, the right-hand side of Eq. (55) decays to zero superpolynomially in the number of pulses, N. The bound (53) then yields, for sufficiently large N,

$$D[\rho_S(T),\rho_S^0(T)] \leq \frac{1}{2}(e^{2JT(\beta T/N^{1/2})^{\log_4 N}} - 1) \leq 2JT(\beta T/N^{1/2})^{\log_4 N}, \quad (57)$$

which shows that the distance between the actual and desired state is maintained arbitrarily well. Distance bounds of this type have also been used in dynamical decoupling applications involving multiple qubits [26,27].

VIII. CONCLUSIONS

We have presented various bounds on the distance between states evolving quantum mechanically, either as closed or as open systems. These bounds are summarized in Theorem 2. We expect our bounds to be useful in a variety of quantum computing or control applications. An undesirable aspect of Eqs. (53) is that the operator norm can diverge if the bath spectrum is unbounded, as is the case, e.g., for an oscillator bath. A brute force solution is the introduction of a high-energy cutoff. However, a more elegant solution is to note [28] (Lemma 8) that every system with energy constraints (such as a bound on the average energy) is essentially supported on a finite-dimensional Hilbert space. An even more satisfactory solution in the unbounded spectrum case is to find a distance bound involving correlation functions. This can be accomplished by performing a perturbative treatment in the system-bath coupling parameter, as is done in the standard derivation of quantum master equations [4,5].

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APPENDIX A: INTERACTION PICTURE

We prove that $\tilde{U}(t,0)$ defined in Eq. (23) satisfies the Schrödinger equation (24) with the interaction picture Hamiltonian defined in Eq. (25). This requires proof since all the Hamiltonians considered are time dependent, whereas usually one only considers the perturbation to be time dependent. To see this we differentiate both sides of Eq. (23), while making use of Eqs. (24) and (25):

$$\begin{aligned}
\frac{dU(t,0)}{dt} &= \frac{d[U_0(t,0)\tilde{U}(t,0)]}{dt} \\
&= \frac{dU_0(t,0)}{dt}\tilde{U}(t,0) + U_0(t,0)\frac{d\tilde{U}(t,0)}{dt} \\
&= -iH_0(t)U_0(t,0)\tilde{U}(t,0) - iU_0(t,0)\tilde{H}(t)\tilde{U}(t,0) \\
&= -iH_0(t)U_0(t,0)\tilde{U}(t,0) \\
&\quad - iU_0(t,0)U_0(t,0)^{\dagger}V(t)U_0(t,0)\tilde{U}(t,0) \\
&= -i[H_0(t)+V(t)]U_0(t,0)\tilde{U}(t,0) \\
&= -iH(t)U(t,0),
\end{aligned}$$

which is the same differential equation as Eq. (21). The initial conditions of the equations are also the same $[U(0,0)=I]$; thus, Eqs. (23)–(25) describe the propagator generated by $H(t)$.

APPENDIX B: DYSON EXPANSION BOUND

We prove Eq. (50). The proof makes use of (1) the triangle inequality, (2) submultiplicativity, and (3) unitary invariance:

$$\begin{aligned}
\|\mathcal{S}(s)-\mathcal{I}\|_{\infty,1} &= \Big\|\sum_{m=1}^{\infty}\mathcal{S}_m(s)\Big\|_{\infty,1} \overset{(1)}{\le} \sum_{m=1}^{\infty}\|\mathcal{S}_m(s)\|_{\infty,1} \\
&= \sum_{m=1}^{\infty}\Big\|\int_0^s ds_1\cdots\int_0^{s_{m-1}} ds_m\prod_{i=1}^{m}\tilde{V}(s_i)\Big\|_{\infty,1} \\
&\overset{(1)}{\le} \sum_{m=1}^{\infty}\int_0^s ds_1\cdots\int_0^{s_{m-1}} ds_m\Big\|\prod_{i=1}^{m}\tilde{V}(s_i)\Big\|_{\infty,1} \\
&\overset{(2)}{\le} \sum_{m=1}^{\infty}\int_0^s ds_1\cdots\int_0^{s_{m-1}} ds_m\prod_{i=1}^{m}\|\tilde{V}(s_i)\|_{\infty,1} \\
&\overset{(3)}{=} \sum_{m=1}^{\infty}\int_0^s ds_1\cdots\int_0^{s_{m-1}} ds_m\|t\,\Delta L(t)\|_{\infty,1}^{m} \\
&= \sum_{m=1}^{\infty}\|t\,\Delta L(t)\|_{\infty,1}^{m}\frac{s^m}{m!} = e^{\|t\,\Delta L(t)s\|_{\infty,1}}-1.
\end{aligned}$$

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